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Methods for reducing biases and errors in regional photochemical model outputs for use in emission reduction and exposure assessments

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HIGHLIGHTS

- Four methods are presented to reduce bias and errors in air quality model output.
- Adjusted modeled concentration time series more closely resemble observations.
- Statistical metrics of adjusted model output are similar to those in observations.
- Adjusted model output can be used for future air quality and exposure assessments.
- Methods presented build confidence in using models for policy and exposure analysis.

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ABSTRACT

In the United States, regional-scale photochemical models are being used to design emission control strategies needed to meet the relevant National Ambient Air Quality Standards (NAAQS) within the framework of the attainment demonstration process. Previous studies have shown that the current generation of regional photochemical models can have large biases and errors in simulating absolute levels of pollutant concentrations. Studies have also revealed that regional air quality models were not always accurately reproducing even the relative changes in ozone air quality stemming from changes in emissions. This paper introduces four approaches to adjust for model bias and errors in order to provide greater confidence for their use in estimating future concentrations as well as using modeled pollutant concentrations in exposure assessments. The four methods considered here are a mean and variance (MV) adjustment, temporal component decomposition (TC) adjustment of modeled concentrations, and two variants of cumulative distribution function (CDF) mapping. These methods were compared against each other as well as against unadjusted model concentrations and a version of the relative response approach based on unadjusted model predictions. The analysis uses ozone concentrations simulated by the Community Multiscale Air Quality (CMAQ) model for the northeastern United States domain for the years 1996–2005. Ensuring that base case conditions are adequately represented through the combined use of observations and model simulations is shown to result in improved estimates of future air quality under changing emissions and meteorological conditions.

1. Introduction

Regional-scale photochemical models are useful tools for forecasting (Eder et al., 2010), regulatory decision-making (USEPA, 2014), and exposure assessments (Garcia et al., 2010; Lin et al., 2013). Forecasts of future air quality enable people to take appropriate precautionary measures to reduce their exposure to high pollution levels (Eder et al., 2010). With respect to exposure assessments, it is desirable to relate air quality to human health at unmonitored locations (Garcia et al., 2010; Lin et al., 2013) and to deal with missing data at monitoring sites (i.e., Junninen et al., 2004). Spatially and temporally dense model outputs, adjusted

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for biases in mean and variability are used for these purposes. Attainment demonstrations use a set of model experiments to assess the magnitude and extent of air pollution and to determine emission reductions needed to meet the National Ambient Air Quality Standards (NAAQS). In particular, models are used to compare past air quality (base case) with model-predicted future conditions. This paper addresses the use of models in attainment demonstrations and exposure assessments.

Before a regional photochemical model is applied in the regulatory setting, USEPA's guidance for the attainment demonstration recommends a thorough evaluation of the model performance for the base case simulation (USEPA, 2014). Sistla et al. (2004), Jones et al. (2005), Pegues et al. (2012), Hogrefe et al. (2012), Kulkarni et al. (2014), and Cohan and Chen (2014) have examined some issues with the use of projected design values in attainment demonstrations. Dennis et al. (2010) provided a framework for performing comprehensive model evaluation, which entails conducting operational (Appel et al., 2007), dynamic (Napelenok et al., 2011), diagnostic (Godowitch et al., 2011), and probabilistic evaluations (Hogrefe and Rao, 2001; Foley et al., 2012; Reich et al., 2013). Also, scientists from North America and Europe have been helping advance the model evaluation framework outlined by Dennis et al. (2010) as part of the Air Quality Modelling Evaluation International Initiative (AQMEII) project (Rao et al., 2011; Galmarini et al., 2012). The AQMEII community is currently focusing on evaluating the performance of coupled meteorology and atmospheric chemistry models (Baklanov et al., 2014) to examine the strengths and limitations of air quality models being used in North America and Europe. In addition, techniques such as Kalman filtering (Delle Monache et al., 2006; Kang et al., 2008, 2010) and spectral decomposition approach (Galmarini et al., 2013) have been used to correct for model bias in air quality forecasting.

It is important to promote model evaluations to establish credibility for air quality models so they can be more confidently used for regulatory decisions. However, despite continual improvement in models, discrepancies between model predictions and observations persist, stemming from both reducible and irreducible errors. In addition, whereas modeled concentrations represent volume-average concentrations, observations reflect point measurements at a given location. Also, the stochastic variations affecting the monitored concentrations are not explicitly modeled in the current regional numerical air quality models. Reducible errors (structural and parametric) are attributable to our inadequate understanding of the relevant atmospheric processes, and errors in model input variables (e.g., emissions, meteorology, boundary conditions, physics and chemistry). Irreducible errors arise from our inability to properly characterize the initial state as well as the stochastic nature of the atmosphere. A critical point to bear in mind is that it is difficult, if not impossible, to specify the atmospheric conditions (i.e., emissions, initial and boundary conditions, meteorology, physics, and chemistry) that real-world observations are seeing in all locations at all times by simulating the base case conditions using air quality models. In consequence, modeled pollutant concentrations often are biased (average observed values are not reproduced) (Simon et al., 2012), exhibit less variability than the corresponding observations (i.e., the distribution of modeled values is often more narrow than that of the observations), and show changes in pollutant levels from the base case that differ from observed changes (Gilliland et al., 2008; Godowitch et al., 2010). One way to address these limitations is to constrain the model output by the observations to ensure that observations and modeled values are starting from the same point so the deviations from the base case can be properly evaluated as emissions and/or meteorology are altered. It should be emphasized that this does not imply that scientific advances for better simulating the interactions of pollutants and transport and fate in the atmosphere are not needed.

In an attempt to better meet the needs of regulatory agencies as well as the health sciences community for regional air quality models, we propose four new methods for bringing the statistical properties (i.e., mean, variance, percentiles) of model predictions into closer harmony with pollutant concentrations observed at monitoring sites. Included are adjustments to the concentration time series (matching the mean and variance of model ozone time series to observations), spectral decomposition of time series (matching the low and high frequency variations in model ozone time series to observations), and two variations of cumulative distribution function (CDF) matching (matching sample CDFs of modeled and observed concentrations, disregarding the time sequence). A ten-year long photochemical model simulation for the northeastern USA is used to assess the performance of these methods. The ability of these methods to reproduce different-year ozone concentrations as well as contemporaneous predictions, that is, same-year ozone concentration time series, is evaluated. The new approaches are compared with absolute model projections and with model-based, relative response factors based on unadjusted model predictions.

2. Data and methods

2.1. A. Model setup

The following is a brief summary of the model set-up used to perform the simulations analyzed in this study. The reader is referred to Hogrefe et al. (2009, 2010) for additional details. The Mesoscale Meteorological Model MM5 (Grell et al., 1994) was used to simulate meteorological conditions for the time period from 1 January 1988 to 31 December 2005. In the current study, we utilize model simulations for the ten year period from 1996 to 2005. The meteorological simulations were performed on two-way nested grids with 36 km and 12 km grid cell sizes covering the northeastern US. Throughout the model simulation, MM5 was nudged towards reanalysis fields from the National Center for Environmental Prediction (NCEP) using four-dimensional data assimilation. All emission processing, including mobile and biogenic sources, was performed within the Sparse Matrix Operator Kernel Emissions (SMOKE) system (Houyoux et al., 2000). Anthropogenic emission inventories for 1988–2005 were compiled from a variety of sources as described in Hogrefe et al. (2009). Various regulatory control programs were implemented for the utility sector (e.g., the acid rain control program, NO_x SIP Call) during the period 1995 to 2005. Also, fleet turnover has contributed to large changes in mobile source emissions and control programs were also implemented for a number of other emission sources. The combined effect of all emission control programs was a decrease of domain-wide anthropogenic NO_x and VOC emission by roughly 24% and 28%, respectively during the 1996–2005 period. Biogenic emissions were estimated with the BEIS3.12 model (Pierce et al., 1998) taking into account MM5 temperature, radiation, and precipitation.

Regional air quality simulations were performed with the Community Multiscale Air Quality (CMAQ) model (Byun and Schere, 2006), version 4.6, rather than CMAQ 4.5.1 that was used in Hogrefe et al. (2009) with the same set of meteorological and emission inputs. Air quality model simulations were performed with two one-way nested grids of 36 km and 12 km, corresponding to the MM5 grids except for a ring of buffer cells. The height of the first model layer was set at 38 m. Gas phase chemistry was represented by the CB-IV mechanism (Gery et al., 1989) while aerosol chemistry was simulated with the “aero3” module. In this study, only results from the 12 km CMAQ simulations were utilized.